Three-Dimensional Simulations of Compressible Turbulence on High-Performance Computing Systems

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Outline of Presentation

- Motivation for research
- Turbulence modeling and Large Eddy Simulation
- Computational approach
- Code performance
- Physical applications

LLNL ASCI Turbulence and Instability Modeling Project

- Develop and validate parameterizations of subgrid-scale (SGS) turbulence effects for compressible, 3-D hydrodynamics applications

- Implement SGS parameterization modules in production codes

- Collaborating with University of Minnesota and Cambridge Hydrodynamics, Inc.

Computing Platforms for Accelerated Strategic Computing Initiative (ASCI)

- **ASCI Red (SNL)**
  - **Intel Pentium Pro 4536-node system**
- **ASCI Blue Pacific (LLNL)**
  - **IBM SP Power-PC 512-node system (to be upgraded to 8-way SMP nodes)**
- **ASCI Blue Mountain (LANL)**
  - **SGI/Cray Origin-2000 MIPS R1000 256-processor NUMA system (to be upgraded to 3072 processors)**

To reduce computational demands, some sort of averaging procedure is often used

$$u(x,y,z,t) = \overline{u}(x,y,z,t) + u'(x,y,z,t)$$

- $\overline{(\ )}$ – **operation may be spatial-, temporal-, or ensemble-averaging**
- **Fewer degrees of freedom are needed since** $\overline{u}$ **is smoother**

Averaging carries a heavy price

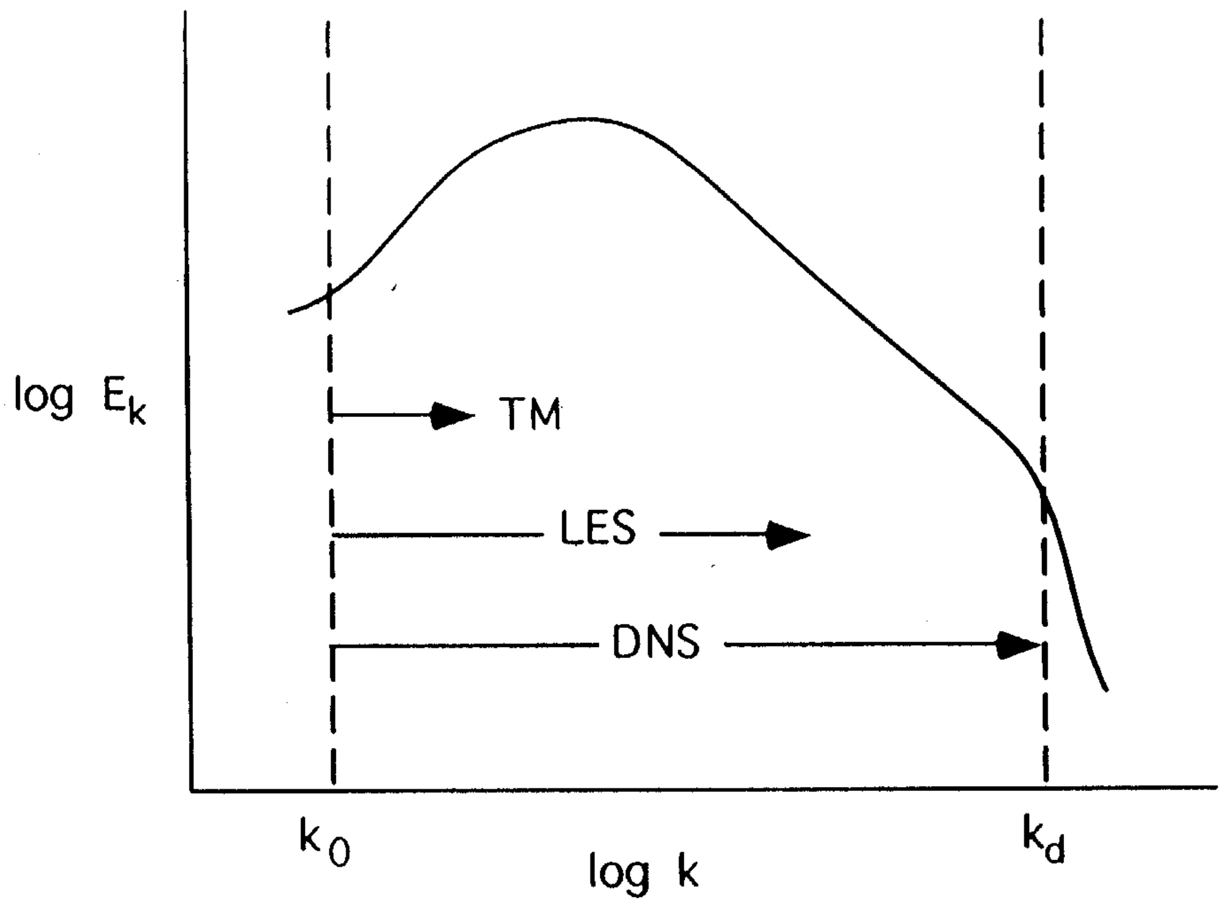
$$\overline{uv} = \overline{(\overline{u} + u')(\overline{v} + v')} = \overline{u}\,\overline{v} + \overline{u'v'}$$

- Equation of motion for $\overline{u}$ contains both $\overline{u}\,\overline{v}$ and new term $\overline{u'v'}$
- In principle, the relation between $\overline{u'v'}$ and $\overline{u}$, $\overline{v}$ is unknown
- Equation of motion for $\overline{u}$ is no longer closed
- Closing the system requires relating second moments to first-order moments

Approaches to the turbulence closure problem

- Ignore it (e.g., use an Euler code; sometimes, for some problems, this is OK!)
- Direct Numerical Simulation (low-to-moderate Reynolds number only)
- Turbulence closure modeling
  - Transport modeling (average over <u>all</u> fluctuating scales)
  - Large Eddy Simulation (average over <u>some</u> fluctuating scales)
- Closure modeling can be based on "first principles," empirical data, phenomenological concepts, or various combinations

Approaches to the turbulence closure problem



Piecewise Parabolic Method (PPM) Code

- Higher-order Godunov method (Colella and Woodward) designed for flows with shocks
- Optional Navier-Stokes terms
- Lagrangian with Eulerian remap
- Directional splitting
- FORTRAN
- 3-D logically rectangular domain decomposition with message-passing
- Communications decomposed into 1-D shifts
- Over 2700 operations per gridpoint per timestep
- 7-Row border (redundant computation to save on communications)

Data Assimilation

- Restart dumps, compressed dumps (2-byte or 1-byte integer)
- Each node produces its own data file
- Data analyzed with PPM tool kit from the University of Minnesota
  - a3d program computes vorticity, power spectra, etc. from individual nodal files
  - a3d can convert to either ascii or bricks-of-bytes (BOB) format
  - Various visualization tools (e.g., PERPATH, BOB) can view BOB format

Comparing Machine Performance

- Common norm of throughput per node/processor must be taken in context
  - processor power
  - processor cost

- ASCI machines are evolving rapidly

Intermachine Comparison

Machine	μs / Δt / point	Mflop / node
LLNL IBM-SP	3.3	25.7
LLNL Cray-T3D	6.4	13.2
Sandia Intel Paragon	21.9	3.9
Sandia Intel ASCI-Red	3.1	27.7
Sandia Intel ASCI-Red	2.4	35.3
Dec Alpha (NE)-1 proc.	23.8	114.0
(Estimate for 32 processors)	(1.1)	(78.8)

32-bit

64-bit

Triply periodic decay problem
128-cubed grid
4 x 4 x 2 domain decomposition (32 processors)

Parallel Efficiency on IBM-SP System

No. of nodes	Decomposition	Local mesh	μs / Δt / meshpoint
8	2 x 2 x 2	64 x 64 x 64	10.5
32	4 x 4 x 2	32 x 32 x 64	3.3
128	4 x 4 x 8	32 x 32 x 16	1.2

- **Drop in parallel efficiency due almost entirely to redundant border computations**

Parallel Efficiency on ASCI-Red System

No. of nodes	Decomposition	Local mesh	µs / Δt / meshpoint
8	2 x 2 x 2	64 x 64 x 64	9.1
32	4 x 4 x 2	32 x 32 x 64	2.4
128	4 x 4 x 8	32 x 32 x 16	0.9

- **Drop in parallel efficiency due almost entirely to redundant border computations**

Scaling with Increasing Problem Size on Intel Paragon

No. of Nodes	Global mesh	Decomp.	Local mesh	μs / Δt / local-point
8	64 x 64 x 64	2 x 2 x 2	32 x 32 x 32	89.3
512	256 x 256 x 256	8 x 8 x 8	32 x 32 x 32	91.6

- Scaling is almost perfect

Rayleigh-Taylor Instability

- Light fluid trying to support heavy fluid
  - air supporting water
  - astrophysics
  - inertial confinement fusion

- Perturbations at fluid interface grow

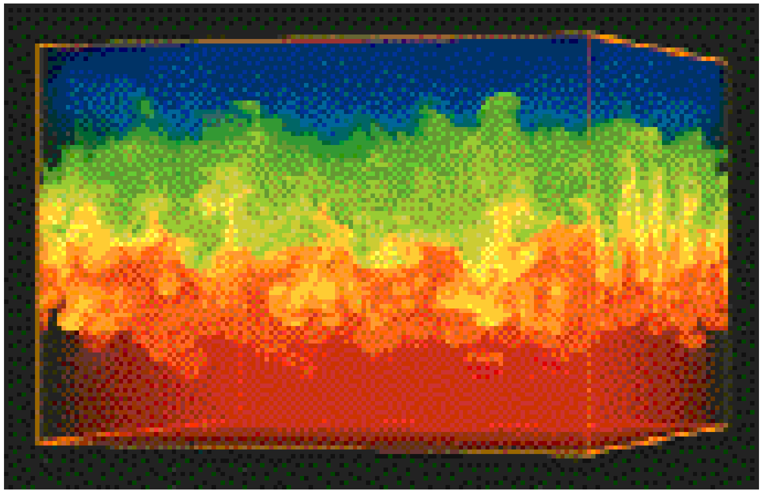
- Mixing layer develops
  - heavier fluid forms spikes as it drops into a lighter fluid
  - lighter fluid forms bubbles as it rises into a heavier fluid

Rayleigh-Taylor Issues of Relevance

- Needed dissipation level for convergence at given mesh resolution
- Dependence of turbulent spectra (energy, vorticity) on wave number
- Mixing rates vs Mach number, Reynolds number, Prandtl number, Atwood number
- Effect of PPM dissipation
- Development and validation of SGS closures

Rayleigh-Taylor Simulation on the ASCI Blue Pacific ID System

- Three-dimensional, compressible Navier-Stokes
- Piecewise Parabolic Method (PPM)
- $512 \times 512 \times 512$ resolution
- Ideal gas, $\gamma = 5 / 3$
- Atwood number = 1 / 3
- Prandtl number (ν / κ) = 1
- Viscosity ($\nu / c_s L_z$) = 4×10^{-5}



Dedication Ceremony Calculation Notes

- Case ran for 84 hours on 128 nodes with one interruption
- 301 frames of volume-rendered temperature produced
- Each frame converted 134 MB of data to 600 x 400 raster image
- 33 restart dumps produced, each requiring 8.3 GB
- Wrote to local disks of IBM-SP; transferred data to mounted disks for postprocessing and storage; combined nodal output files into single file

Shock-Turbulence Interaction

- Study interaction of shock wave with pre-existing 3-D turbulence
  - multiple shocks passing through interface of different density materials
- How does shock affect turbulence strength, spectrum, anisotropy, rate of shock propagation?
- Development and validation of SGS closures

Physical Scenario

- Initially run 3-D decay problem with triply periodic boundary conditions
- After turbulence decays to lower level, impose inflow shock conditions on left edge
- Observe unshocked turbulent region to right of shock, shocked turbulent region behind shock, and quiescent inflow near left edge
- These are pure Euler calculations at 256-cubed resolution

Shock-Turbulence Results

- Shock strongly enhances and anisotropizes turbulence
- Mach 6 effects stronger than Mach 2 effects
- Simulations appear to resolve portion of inertial range
- Shock slightly sped up by presence of turbulence

Toward the Future

- PPM is effective tool for simulating 3-D compressible turbulence
- High resolution (up to billions of zones) will be needed to develop and validate SGS closures
- Robust I/O and post processing environment needed for data assimilation
- We will need a lot of computer time (and disk)